

1) To solve an equation when there is no formula for the exact solution available, we can use an approximation method, such as an **iteration method**. This is a method in which we start from an initial guess  $x_0$  (which may be poor) and compute step by step (in general better and better) approximations  $x_1, x_2, \dots$  of an unknown solution.

2) By some algebraic steps we transform (1) into the form

$$(2) \quad x = g(x)$$

Then we choose an  $x_0$  and compute  $x_1 = g(x_0)$ ,  $x_2 = g(x_1)$ , and in general

$$(3) \quad x_{n+1} = g(x_n) \quad (n=0, 1, \dots)$$

A solution of (2) is called a **fixed point** of  $g$ , motivating the name of the method. This is a solution of (1), since from  $x = g(x)$  we can return to the original form  $f(x) = 0$ . From (1) we may get several different forms of (2). The behavior of corresponding iterative sequences  $x_0, x_1, \dots$  may differ, in particular, with respect to their speed of convergence. Indeed, some of them may not converge at all. Let us illustrate these facts with a simple example.

3) (a)  $\frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$  :  $a=1, b=-3, c=1$  :  $x_1 = \frac{3 + \sqrt{9 - 4(1)(1)}}{2(1)}, x_2 = \frac{3 - \sqrt{9 - 4(1)(1)}}{2(1)}$   
 $x_1 = \frac{3 + \sqrt{5}}{2} = 1.5 + \sqrt{1.25}, x_2 = \frac{3 - \sqrt{5}}{2} = 1.5 - \sqrt{1.25}$

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(b)  $f(x) = x^2 - 3x + 1 = 0$

$$\begin{aligned} x^2 - 3x + 1 &= 0 \Rightarrow x^2 + 1 = 3x \Rightarrow \frac{1}{3}(x^2 + 1) = x \quad \text{Thus: } x_{n+1} = \frac{1}{3}(x_n^2 + 1) \\ x^2 - 3x + 1 &= 0 \Rightarrow x^2 = 3x - 1 \Rightarrow x = 3 - \frac{1}{x} \quad \text{Thus: } x_{n+1} = 3 - \frac{1}{x_n} \end{aligned}$$

(c) Our figures show the following. In the lower part of Fig. 426a the slope of  $g_1(x)$  is less than the slope of  $y=x$ , which is 1, thus  $|g_1'(x)| < 1$ , and we seem to have convergence. In the upper part,  $g_1(x)$  is steeper ( $g_1'(x) > 1$ ) and we have divergence. In Fig. 426b the slope of  $g_2(x)$  is less near the intersection point ( $x=2.618$ , fixed point of  $g_2$ , solution of  $f(x)=0$ ), and both sequences seem to converge. From all this we conclude that convergence seems to depend on the fact that, in a neighborhood of a solution, the curve of  $g(x)$  is less steep than the straight line  $y=x$ , and we shall now see that this condition  $|g'(x)| < 1$  (=slope of  $y=x$ ) is sufficient for convergence.

4) **Theorem 2: Convergence of Fixed-Point Iteration**

Let  $x = s$  be a solution of  $x = g(x)$  and suppose that  $g$  has a continuous derivative in some interval  $J$  containing  $s$ . Then, if  $|g'(x)| \leq k < 1$  in  $J$ , the iteration process defined by (3) converges for any  $x_0$  in  $J$ . The limit of the sequence  $\{x_n\}$  is  $s$ .

5) **Algorithm Newton ( $f, f', x_0, \epsilon, N$ )**

This algorithm computes a solution of  $f(x) = 0$  given an initial approximation  $x_0$  (starting value of the iteration.) Here the function  $f(x)$  is continuous and has a continuous derivative  $f'(x)$ .

**INPUT:**  $f, f'$ , initial approximation  $x_0$ , tolerance  $\epsilon > 0$ , maximum number of iterations  $N$ .

**OUTPUT:** Approximate Solution  $x_n$  ( $n \leq N$ ) or message of failure.

For  $n=0, 1, 2, \dots, N-1$  do:

1      Compute  $f'(x_n)$

2      IF  $f'(x_n) = 0$  then OUTPUT "Failure." Stop.  
[Procedure completed unsuccessfully]

3      Else Compute

$$(5) \quad x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

4      IF  $|x_{n+1} - x_n| \leq \epsilon |x_{n+1}|$  then OUTPUT  $x_{n+1}$ . Stop.  
[Procedure completed successfully]

5      OUTPUT "Failure". Stop.  
[Procedure completed unsuccessfully after  $N$  iterations]

END

END Newton

6) The inequality in line 4 is a **termination criterion**. If the sequence of the  $x_n$  converges and the criterion holds, we have reached the desired accuracy and stop. Note that this is just a form of the relative error test. It ensures that the result has the desired number of significant digits. If  $|x_{n+1}| = 0$ , the condition is satisfied if and only if  $x_{n+1} = x_n = 0$ , otherwise  $|x_{n+1} - x_n|$  must be sufficiently small. The factor  $|x_{n+1}|$  is needed in the case of zeros of very small (or very large) absolute value because of the high density (or of the scarcity) of machine numbers for those  $x$ .

7) Line 5 gives another termination criterion and is needed because Newton's method may diverge or, due to a poor choice of  $x_0$ , may not reach the desired accuracy by a reasonable number of iterations. Then we may try another  $x_0$ . If  $f(x) = 0$  has more than one solution, different choices of  $x_0$  may produce different solutions. Also, an iterative sequence may sometimes converge to a solution different from the expected one.

8) **Example 5** Newton's Method Applied to an Algebraic Equation

Apply Newton's method to the equation  $f(x) = x^3 + x - 1 = 0$ .

Solution. From (5) we have

$$x_{n+1} = x_n - \frac{x_n^3 + x_n - 1}{3x_n^2 + 1} = \frac{2x_n^3 + 1}{3x_n^2 + 1}.$$

Starting from  $x_0=1$ , we obtain

$$x_1 = 0.780000, x_2 = 0.686047, x_3 = 0.682340, x_4 = 0.682328$$

Where  $x_4$  has the error  $-1 \cdot 10^{-6}$ . A comparison with Example 2 shows that the present convergence is much more rapid. This may motivate the concept of the order of an iteration process, to be discussed next.

### 9) Order of an Iteration Method. Speed of Convergence.

The quality of an iteration method may be characterized by the speed of convergence, as follows.

Let  $x_{n+1} = g(x_n)$  define an iteration method, and let  $x_n$  approximate a solution  $s$  of  $x = g(x)$ . Then  $x_n = s - E_n$ , where  $E_n$  is the error of  $x_n$ . Suppose that  $g$  is differentiable a number of times, so that the Taylor formula gives

$$(6) \quad x_{n+1} = g(x_n) = g(s) + g'(s)(x_n - s) + \frac{1}{2}g''(s)(x_n - s)^2 + \dots = g(s) - g'(s)E_n + \frac{1}{2}g''(s)E_n^2 + \dots$$

The exponent of  $E_n$  in the first nonvanishing term after  $g(s)$  is called the **order** of the iteration process defined by  $g$ . The order measures the speed of convergence.

To see this, subtract  $g(s) = s$  on both sides of (6). Then on the left you get  $x_{n+1} - s = -E_{n+1}$ , where  $E_{n+1}$  is the error of  $x_{n+1}$ . And on the right the remaining expression equals approximately its first nonzero term because  $|E_n|$  is small in the case of converge. Thus

- (7)
- (a)  $E_{n+1} \approx -g'(s)E_n$  in the case of first order,
  - (b)  $E_{n+1} \approx -\frac{1}{2}g''(s)E_n^2$  in the case of second order, etc.

Thus if  $E_n = 10^{-k}$  in some step, then for second order,  $E_{n+1} = C \cdot (10^{-k})^2 = C \cdot 10^{-2k}$ , so that the number of significant digits is about doubled in each step.

### 10) Theorem 2: Second-order Convergence of Newton's Method

If  $f(x)$  is three times differentiable and  $f'$  and  $f''$  are not zero at a solution  $s$  of  $f(x)=0$ , then for  $x_0$  sufficiently close to  $s$ , Newton's method is of second order.

**Comments:** For Newton's method, (7b) becomes, by (8\*),

$$(9) \quad E_{n+1} \approx -\frac{f''(s)}{2f'(s)} E_n^2$$

For the rapid convergence of the method indicated in Theorem 2 it is important that  $s$  be a simple zero of  $f(x)$  (thus  $f'(s) \neq 0$ ) and that  $x_0$  be close to  $s$ , because in Taylor's formula we took only the linear term [see (5\*)], assuming the quadratic term to be negligibly small. (With a bad  $x_0$  the method may even diverge!)

### 11) Difficulties in Newton's Method:

Difficulties may arise if  $|f'(x)|$  is very small near a solution  $s$  of  $f(x)=0$ . In this case of  $f(x)=0$ , we call  $f(x)$  **ill-conditioned**.

### 12) Secant Method for Solving $f(x)=0$

Newton's method is very powerful but has the disadvantage that the derivative  $f'$  may sometimes be a far more difficult expression than  $f$  itself and its evaluation therefore computationally expensive. This situation suggests the idea of replacing the derivative

with the difference quotient

$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

Then instead of (5) we have the formula of the popular Secant method

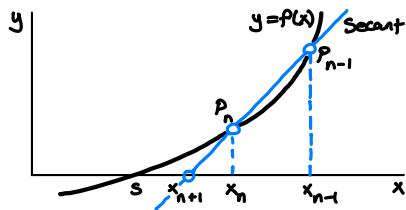


Fig. 429. Secant method

(10)

$$x_{n+1} = x_n - \frac{f(x_n)}{f(x_n) - f(x_{n-1})} \cdot x_n - x_{n-1}$$

Geometrically, we intersect the x-axis at  $x_{n+1}$  with the secant of  $f(x)$  passing through  $P_{n-1}$  and  $P_n$  in Fig. 429. We need two starting values  $x_0$  and  $x_1$ . Evaluation of derivatives is now avoided. It can be shown that convergence is **Superlinear** (that is, more rapid than linear,  $|x_{n+1}| \approx \text{Const} \cdot |x_n|^{1.62}$ ; See [E5] in App. I), almost quadratic like Newton's method. The algorithm is similar to that of Newton's method, as the student may show.

**CAUTION!** It is not good to write (10) as

$$x_{n+1} = \frac{x_{n-1}f(x_n) - x_nf(x_{n-1})}{f(x_n) - f(x_{n-1})}$$

because this may lead to loss of significant digits if  $x_n$  and  $x_{n-1}$  are about equal. (Can you see this from the formula?)